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Thomas Aktor, Antti-Pekka Jauho and Stephen R. Power

Introduction

Gating of individual atoms in graphene would allow extremely precise control of current flow. In practice, however, this is very difficult to achieve. In this work we investigate whether doping or spatially restricted gating can be used to achieve similar control. Two systems are considered:

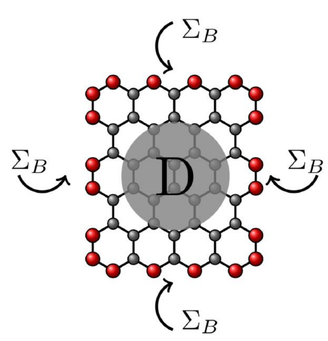
- Sublattice asymmetric doping within a region in a pristine graphene sheet [1,2].
- Sublattice symmetric gated region in a pristine graphene sheet [4].

Methods

We use:

- A 1NN tight binding model.
- The **Patched Green's Functions** (PGF) method [3]
  - The PGF is explained in the right coloumn.
- A simple onsite energy shift for dopants

Schematic of PGF



Why Patched Green's Functions?

When computing the effect of disorder, the main challenges are the "low" number of atoms that can be considered at once, and the corresponding boundary condtions, typically edges or periodicity.

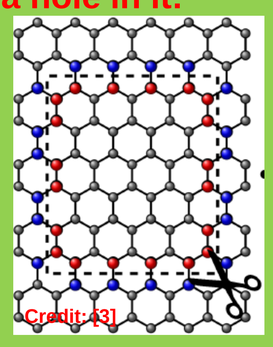
An alternative is to use the **Patched Green's Functions** method [3], where the boundary conditions are replaced by a boundary selfenergy.

This enables one to effectivly imbed a region into a periodic material, as long as a simple expression for the real-space Green's Functions is available.

How does it work?

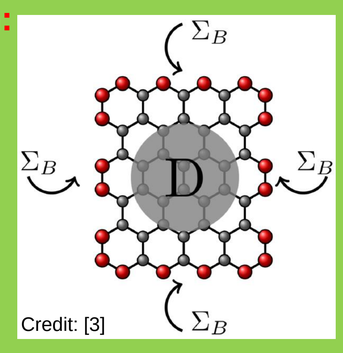
Step 1:

Take a pristine graphene sheet and cut a hole in it:



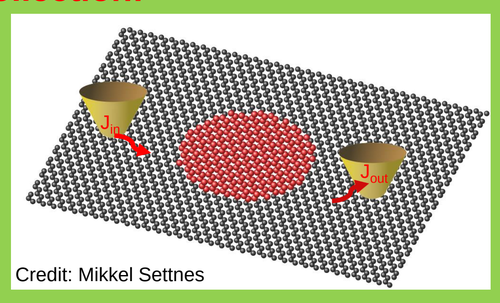
Step 2:

Embed a device in the cut-out region:



Step 3:

Probes for current injection and collection:



Step 4:

Apply equations:

B,D refers to the boundary and device respectivly

$$G_{D,D}^{(con)} = \left(E1 - H_{D,D} - \Sigma_B\right)^{-1}$$

The device Hamiltonian is divided in parts and constructed recursively.

$$\Sigma_B = V_{D,B} G_{B,B}^{(dis)} V_{B,D}$$

$$G_{B,B}^{(dis)} = \left(1 - G_{B,D}^{(0)} V_{D,B}\right)^{-1} G_{B,B}^{(0)}$$

(0) refers to the pristine material.

$$J_{i,j}^{L} = -H_{ij}\,\mathrm{Im}[G^a \Gamma^L G^r]_{ij}/\hbar$$

Here i and j refers to specific sites. The a and r are the advanced and retarded GF's respectively (of the fully connected)

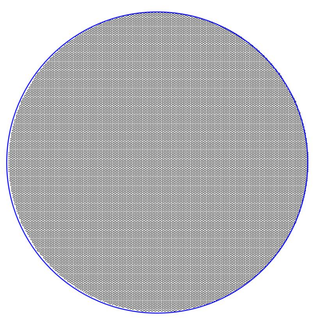
Sublattice symmetric potential

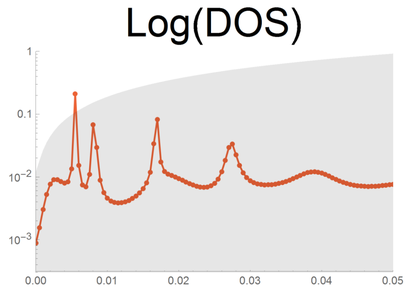
The onsite potential is shifted in both sublattices, with an **average** change (keeping the shift times concentration constant) of: $\epsilon_A = \epsilon_B = 0.1|t|$, for a varying concentration of atoms ($c = 1.0, 0.5, 0.2$) within a circular region of radius 20nm. The positive energies are the most interesting .

$E_{onsite} \neq 0$

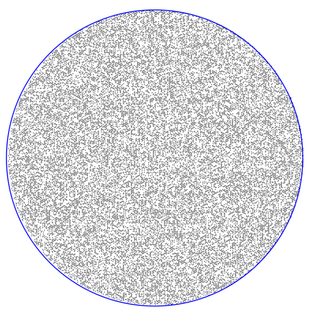
Density of states (shaded region is the pristine version)

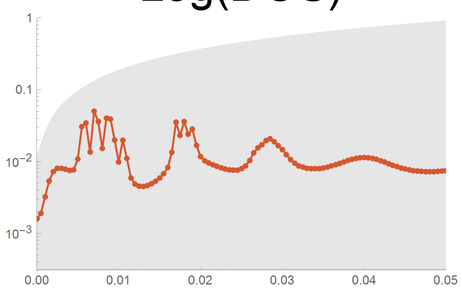
- $c = 1.0$



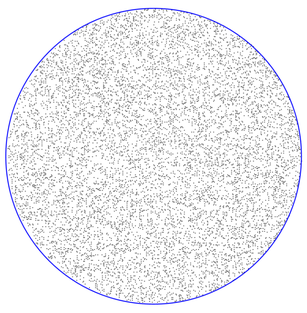


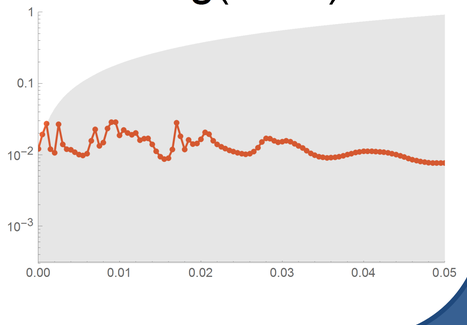
- $c = 0.5$





- $c = 0.2$





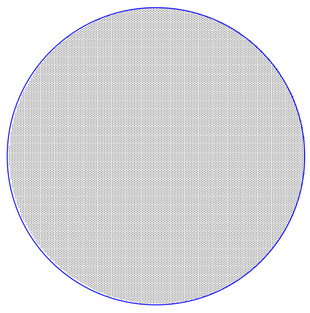
Sublattice asymmetric potential

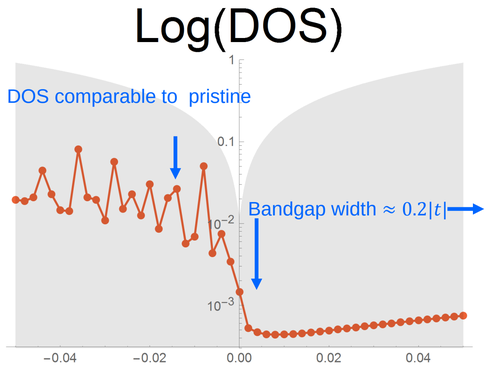
The onsite potential is shifted in one of the sublattices, with an **average** change (keeping the shift times concentration constant) of : $\epsilon_A = 0.2|t|$; $\epsilon_B = 0$, for a varying concentration of A-atoms ($c_A = 1.0, 0.5, 0.2$) within a circular region of radius 20nm.

$E_{onsite} \neq 0$

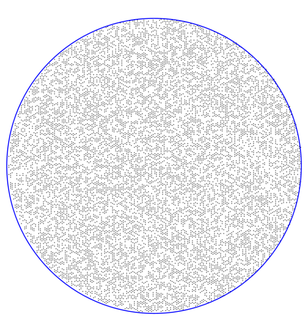
Density of states (shaded region is the pristine version)

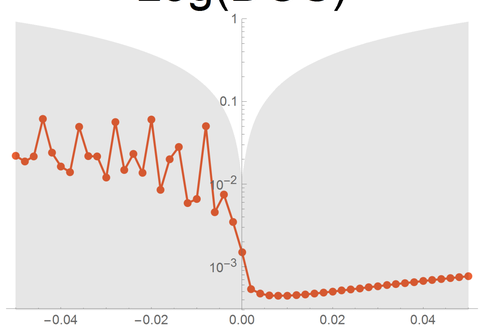
- $c_A = 1.0$



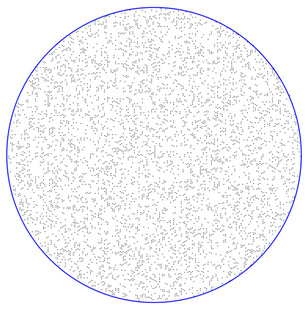


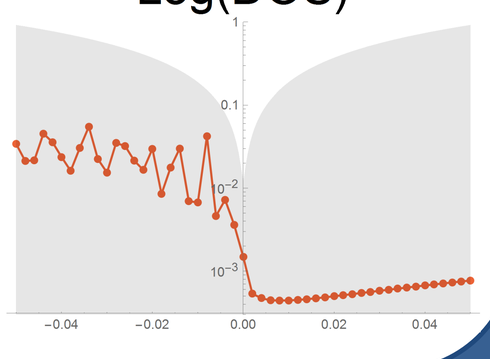
- $c_A = 0.5$





- $c_A = 0.2$





Sublattice imbalance

- Asymmetric doping of graphene results in different **average** potentials on the A and B sublattices

$$H = \begin{pmatrix} \epsilon_A & -tf(\boldsymbol{k}) \\ -tf(\boldsymbol{k})^* & \epsilon_B \end{pmatrix}$$

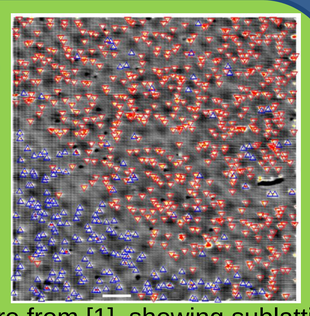


Figure from [1], showing sublattice imbalance in experiments

- Energy spectrum:

$$\epsilon_{\pm}(\boldsymbol{k}) = \frac{1}{2}(\epsilon_A + \epsilon_B) \pm \frac{1}{2}\sqrt{(\epsilon_A - \epsilon_B)^2 + 4t^2|f(\boldsymbol{k})|^2}$$

with a bandgap $|\epsilon_A - \epsilon_B|$. $\frac{|\epsilon_A - \epsilon_B|}{2}$ is also called a **mass term**.

Fact box

Green's Function of Graphene

Fact box

- The 1NN tight binding model graphene pristine Hamiltonian.

$$H^{(0)} = \begin{pmatrix} 0 & -tf(\boldsymbol{k}) \\ -tf(\boldsymbol{k})^* & 0 \end{pmatrix}, \quad f(k) = 1 + e^{-i\boldsymbol{k}\cdot\boldsymbol{a_1}} + e^{-i\boldsymbol{k}\cdot\boldsymbol{a_2}}$$

- The Green's Function

$$G^{(0)}(z, \boldsymbol{r_i}, \boldsymbol{r_j}) = \frac{1}{\Omega_{BZ}} \int d^2\boldsymbol{k} \frac{N_{ij}(z,\boldsymbol{k}) e^{i\boldsymbol{k}\cdot(\boldsymbol{r_j} - \boldsymbol{r_i})}}{z^2 - t^2|f(\boldsymbol{k})|^2} \qquad N_{ij}(z, \boldsymbol{k}) = \begin{cases} z \\ tf(\boldsymbol{k}) \\ tf^*(\boldsymbol{k}) \end{cases}$$

Depending on the sublattice of i,j

- One of the k integrals can be done analytically [4], leaving one to be calculated numerically

Conclusions

- The key features of the DOS for the asymmetrically doped dot are largely independent of c_A
- The key features of the DOS for the uniformly gated dot are very dependent on the concentration. The peaks associated with the vortex behavior get completely smeared out.

Outlook

- The **Patched Green's Functions** method allows for calculations for non-periodic yet infinite system, in particular in graphene.
- Using the boundary to account for lost current one can calculate, not only the transmission, but the physical current between two leads.
- Combinations of localized disorder, such as doping or vacancies can be explored.

References

[1]: A. Zabet-Khosousi *et al. (*2014*)JACS.*, Vol. 136, 4, 1391-1397.
[2]: Zhao *et al*. (2011). *Science*, *333*(6045), 999–1003.
[3]: Settnes, M. *et al.* (2015). *Physical Review B*, *91*(12), 125408.
[4]: Heinisch, R. L., Bronold, F. X., & Fehske, H. (2013).. *Physical Review B, 87*(15), 155409.

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